

Full counting statistics and the Edgeworth series for matrix product states

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We consider full counting statistics of spin in matrix product states. In particular, we study the approach to gaussian distribution for magnetization. We derive the asymptotic corrections to the central limit theorem for magnetization distribution for finite but large blocks in analogy to the Edgeworth series. We also show how central limit theorem like behavior is modified for certain states with topological characteristics such as the AKLT state.

With the advantage of precision experiments in condensed matter physics, it is now possible to probe the nature of correlated quantum systems to ever higher degrees of detail and precision. This is especially apparent in cold atom systems, where in addition to refined correlation measurements, we also have fine control of the Hamiltonian parameters themselves. One of the most useful ways of studying detailed correlations in the intermediate regime between the macroscopic, thermodynamic properties, and the microscopic, atom by atom level, is through the full counting statistics functions. These describe the full probability distribution of suitable observables, such as the magnetization of a block of spins in a spin chain or the total excess charge flowing through a quantum point contact.

The full counting statistics function (FCS) contains detailed information about the properties of the state. It has been a useful tool to analyze quantum states, from its original appearance in quantum optics, in the theory of photon detectors [1, 2] in quantum optics to counting statistics of electrons in mesoscopic systems introduced by Levitov and Lesovik [3]. The full counting statistics has studied in numerous electronic systems theoretically [4–8] as well as in experiments [9, 10]. The utility of full counting statistics for cold atoms was pointed out in [11]. It has also been demonstrated that in certain cases counting statistics may be used to characterize block entanglement entropy in fermions states and spin states [12–14]. Recently, the analyticity properties of the “bulk” component of the full counting statistics in classical Ising and quantum XY spin chains has been used as an alternative characterization of phases [15].

Here, we explore the quantum noise in an important class of 1d states, the so called matrix product states (MPS) [16]. Such states appear as the ground states of frustration free Hamiltonians, and are especially useful as variational states to study other 1d quantum systems. MPS posses convenient properties that allow a thorough study of correlations and fluctuations in them, for example, an analogue of the Wick’s theorem has been demonstrated for generic translationally invariant MPS in [17]. Finally, we remark that our results also hold for non quantum states as long as the probability distribution of certain measurements may be described in terms analogous to MPS, a prominent example for which is the

exact solution of the 1D asymmetric exclusion process [18], in a recent paper, the full counting statistics for the asymmetric exclusion model was considered in [19].

Here, we concentrate on the corrections to central limit theorem (CLT) like behavior of the full counting statistics. The central limit theorem is a description of the statistics of averages of independent random variables, stating that properly weighted average tend to a Gaussian distribution when the number of random variables is large. Since the correlation length in a MPS, say, is finite, one may expect gaussian like behavior for the magnetization of large blocks of spins. We find that the simple structure of the MPS allows us to not only do this but much more: we can controllably identify how the central limit of magnetization is reached, what are the main corrections (a consequence of entanglement in the system) and show how CLT may sometimes completely fail in cases of topological states.

The distribution of magnetization approach to Gaussian behavior at large spin blocks is substantially more intricate for the MPS as opposed to independent random variables. To address this behavior we concentrate on deriving the asymptotic probability distribution and corrections to it. While in many cases, even when the distribution seems Gaussian in the infinite block size limit, the corrections due to finite block size are modified. Such corrections, are described, for independent, identically distributed variables using various asymptotic series such as the Gram-Charlier A series and the Edgeworth series [20, 21]. The Edgeworth series has been extensively studied in the mathematical literature, with the focus on ensuring its applicability when dealing with random identically distributed variables, which may have divergent moments, see e. g. [22–24].

Here, we derive an expression for the asymptotic corrections to the central limit error function of MPS in analogy to the asymptotic Edgeworth series. We start by deriving formulas for the full counting statistics generating function. For an extensive review of MPS their properties, and their relation to DMRG see [25, 26]. MPS have been shown to be extremely well suitable for approximation of ground states of gapped Hamiltonian [27, 28]. Let us consider a MPS with periodic boundary conditions on N spins, defined as follows:

$$\psi = \sum_{\{\sigma\}} \text{Tr} (A_{\sigma_1} A_{\sigma_2} \dots A_{\sigma_N}) |\sigma_1 \sigma_2 \dots \sigma_N\rangle \quad (1)$$

where $A_\sigma \in \{A_1, \dots, A_S\}$, S is the spin index, and $\sigma_1 \in \{1, \dots, S\}$. The matrices A are of size $D \times D$, where D is called the bond dimension.

To express the full counting statistics of the spin variable σ , we define:

$$E(\lambda) = \sum_\sigma e^{i\lambda\sigma} \bar{A}_\sigma \otimes A_\sigma. \quad (2)$$

The full counting statistics generating function of the magnetization of a block of l sites is then given by

$$\begin{aligned} \chi(\lambda; l; N) &\equiv \sum_n \text{prob}(\text{total spin of block} = n) e^{i\lambda n} = \\ &= \left\langle e^{i\lambda \hat{S}_l} \right\rangle = \frac{\text{Tr} E(\lambda)^l E(0)^{N-l}}{\text{Tr} E(0)^N}. \end{aligned} \quad (3)$$

Here $\hat{S}_l = \sum_{i=1}^l \hat{\sigma}_i$ where $\hat{\sigma}_i$ is a spin operator at site i . When considering the thermodynamic limit, we add, as is usual, the demand that:

$$\sum_{\sigma=1}^S A_\sigma A_\sigma^+ = I \quad (4)$$

This ensures that the largest eigenvalue of $E(0)$ is $\lambda = 1$. In addition, when dealing with problems in the thermodynamic limit we assume this largest eigenvalue is non degenerate. In the thermodynamic limit, we define:

$$\chi(\lambda; l) \equiv \lim_{N \rightarrow \infty} \chi(\lambda; l; N) \quad (5)$$

The existence of the limit is assured by the conditions above. To compute $\chi(\lambda; l)$ we define $P(\lambda)$ to be the matrix which brings $E(\lambda)$ to its Jordan form, with Jordan blocks J_k arranged such that the block with the largest eigenvalue is J_1 . Note that the number of blocks as well as eigenvalues depend on λ . We have:

$$E(\lambda)^l = P(\lambda) (\oplus_{k=1} J_k^l) P^{-1}(\lambda) \quad (6)$$

We note that if there is no degeneracy,

$$E(0)^N \rightarrow P(0) |1\rangle \langle 1| P^{-1}(0) \quad (7)$$

Therefore the full counting statistics function is given by:

$$\chi(\lambda; l) = \langle 1 | P^{-1}(0) P(\lambda) (\oplus_{k=1} J_k^l) P^{-1}(\lambda) P(0) | 1 \rangle \quad (8)$$

Let $\alpha_k(\lambda)$ be the diagonal value of J_k . We can compute explicitly the power of a Jordan block, obtaining after some algebra the formula:

$$\chi(\lambda, l) = \sum_{k=1}^{d_k} \sum_{i=1}^{\min(l, d_k) - i} \sum_{\nu=0}^{d_k - i} C_\nu^l Q_{k,i,\nu} \alpha_k^{l-\nu} \quad (9)$$

where C_ν^l are the binomial coefficients, d_k the dimension of Jordan block k and

$$\begin{aligned} Q_{k,i,\nu}(\lambda) &= \langle i + \nu + \sum_{n=0}^{k-1} d_n | P^{-1}(\lambda) P(0) | 1 \rangle \times \\ &\langle 1 | P^{-1}(0) P(\lambda) | i + \nu + \sum_{n=0}^{k-1} d_n \rangle. \end{aligned} \quad (10)$$

Note that in (9), $Q_{k,i,\nu}$ as well as the limits in the sum depend on λ implicitly.

Since the largest eigenvalue 1 of $E(0)$ is non-degeneracy, we have that $Q_{1,1,0}(0) = 1$ and $Q_{k,i,\nu}(0) = 0$ for all other value of k, i, ν . It is also important note that since, generically, eigenvalues do not cross, we expect that we may set $d_k = 1, \nu = 0$ in (9) for almost all values of $\lambda \in [-\pi, \pi]$, unless some special symmetry or constraint is present.

Let us now consider the limit of large block size l . As with any thermodynamic quantity, computed in a system with finite correlation length, we expect a gaussian distribution of observables according to the CLT. For a matrix product state, of course, the spins are not independent, and so the central limit distribution receives contributions from two types of corrections: due to correlations and due to finite size. Below we establish this behavior and derive the appropriate asymptotic description of the probability distribution for large but finite blocks.

In the limit of large l , if the largest eigenvalue of the matrix $E(\lambda)$ is non degenerate, $E(\lambda)^l$ is dominated by the largest eigenvalue $\alpha_1(\lambda)$ and we may write that:

$$\chi(\lambda; l) \sim \chi_0(\lambda) \chi_1(\lambda)^l \quad \text{as } l \rightarrow \infty \quad (11)$$

where:

$$\chi_1(\lambda) = \alpha_1(\lambda) ; \quad \chi_0(\lambda) = Q_{1,1,0}(\lambda)$$

It is possible to take into account the corrections due to the smaller eigenvalues of $E(\lambda)$ as well, giving additional exponentially small corrections.

We are now in position to describe the probability distribution of block magnetization. Let us define:

$$\hat{M}_l = \frac{1}{\sqrt{l}} \frac{\hat{S}_l - l\mu(l)}{\text{var}(\sigma, l)} \quad (12)$$

where $\mu(l)$ is the average magnetization per site, and $\text{var}(\sigma, l)$ is the variance *per site*. We note that since the spin variables on different sites are not independent, both $\mu(l)$ and $\text{var}(\sigma, l)$ depend explicitly on the size of the block. Let

$$F_l(M) = \text{Prob}(\hat{M}_l \leq M) \quad (13)$$

be the probability distribution of measuring \hat{M}_l . To find $F_l(M)$, we now focus on the FCS for \hat{M}_l , defined as:

$$\chi_M(\lambda; l) = \langle e^{i\lambda \hat{M}_l} \rangle. \quad (14)$$

Since we assume that the largest eigenvalue of $E(\lambda)$ is non degenerate at $\lambda = 0$, this eigenvalue is analytic in a neighborhood of $\lambda = 0$. Indeed both $\chi_0(\lambda), \chi_1(\lambda)$ are analytic in the domain $\lambda \leq |\lambda_*|$ where λ_* is the smallest λ (in the complex plane) for which the largest eigenvalue of

$E(\lambda)$ becomes degenerate (see, e.g. [29]). We can therefore expand $\log(\chi_1(\lambda)), \log(\chi_0(\lambda))$ near $\lambda = 0$. Noting that $\chi_0(\lambda) = \chi_1(\lambda) = 1$ we have the "cumulants" κ_r and ξ_r in:

$$\begin{aligned} \log(\chi_0(\lambda)) &= \sum_{r=1}^{\infty} \frac{\xi^r (i\lambda)^r}{r!} \\ \log(\chi_1(\lambda)) &= \sum_{r=1}^{\infty} \frac{\kappa^r (i\lambda)^r}{r!}. \end{aligned} \quad (15)$$

We see that for a block of l spins, $\mu(l) = \langle \sigma \rangle = \kappa_1 + \xi_1/l$, and $\text{var}(\sigma, l) = \sqrt{\langle \sigma^2 \rangle - \langle \sigma \rangle^2} = \sqrt{\kappa_2 + \xi_2/l}$. We also recognize χ_0 as boundary (or "Edge") term that characterize the effect of the rest of the chain on the chosen l spins, and χ_1 as the bulk term that is not effected by other spins.

In this paper χ_1 plays, formally, the role of the local independent random variable in the usual derivation of the central limit theorem. However, it is important to note that in a generic MPS, χ_1 is not the full counting statistics of a valid probability distribution. Indeed, for that, the associated distribution, given by the Fourier transform of χ_1 must be a positive real function.

Let us briefly explore how close χ_1 is to a valid probability distribution. To do so we write the counting statistics of a block of size 1 as:

$$\chi(\lambda, 1) = \chi_1(\lambda) + \chi_\delta(\lambda), \quad (16)$$

and define the pseudo-probabilities:

$$\tilde{p}_{n,i} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\lambda \chi_i(\lambda) e^{-i\lambda n} \quad ; \quad i = 1, \delta. \quad (17)$$

Associated with the various eigenvalues of the $\chi_1(\lambda), \chi_\delta(\lambda)$. Thus $\tilde{p}_{n,1}$ is the effective probability distribution which would have generated the asymptotic behavior described by the central limit behavior. We can establish the following properties:

1) From the definition of χ_1 , we can immediately infer that the associated distribution is discrete.

Indeed, observe that since $E(\lambda)$ is periodic, we can choose $\chi_1(\lambda)$ to be periodic: $\chi_1(\lambda) = \chi_1(\lambda + 2\pi)$, which is associated with discrete, integer, spins.

2) The distribution is real (however it is in general not necessarily positive).

The second property is established by noting that:

$$E(-\lambda) = \tau \overline{E(\lambda)} \tau \quad (18)$$

where τ swaps $v_1 \otimes v_2 \rightarrow v_2 \otimes v_1$. Therefore

$$\text{spec} E(-\lambda) = \text{spec} \overline{E(\lambda)} \quad (19)$$

and, in particular $\chi_1(-\lambda) = \chi_1^*(\lambda)$, ensuring the Fourier transform is real. It is, however, in general not associated with a probability distribution, since the Fourier transform is, in general, not strictly positive.

3) $\sum_n \tilde{p}_{n,1} = 1$ and $\sum_n \tilde{p}_{n,\delta} = 0$. To prove this note that $\chi_\delta(0) = 0$ since $\chi(0, 1) = \chi_1(0) = 1$. Now use that $\sum_n \tilde{p}_{n,\delta} = \chi_\delta(0)$.

We now proceed to derive the Edgeworth series for our MPS. Using the definition (12) and eq. (11), we can find the cumulants for the distribution of \hat{M}_l :

$$\begin{aligned} \log \chi_M(\lambda; l) &= \frac{(i\lambda)^2}{2} + \frac{(i\lambda)^3 (l\kappa_3 + \xi_3)}{6(l\kappa_2 + \xi_2)^{3/2}} \\ &+ \frac{(i\lambda)^4 (l\kappa_4 + \xi_4)}{24(l\kappa_2 + \xi_2)^2} + \frac{(i\lambda)^5 (l\kappa_5 + \xi_5)}{120(l\kappa_2 + \xi_2)^{5/2}} + \dots \end{aligned} \quad (20)$$

We note that for the normal distribution, we have:

$$\log(\phi(\lambda)) = \frac{(i\lambda)^2}{2} \quad (21)$$

Combine the two equations, and collect terms according to the power of l , we have

$$\begin{aligned} \log \frac{\chi_M(\lambda)}{\phi(\lambda)} &= \frac{1}{l^{1/2}} \frac{(i\lambda)^3 \kappa_3}{6\kappa_2^{3/2}} + \frac{1}{l} \frac{(i\lambda)^4 \kappa_4}{24\kappa_2^2} \\ &+ \frac{1}{l^{3/2}} \left[\frac{(i\lambda)^5 \kappa_5}{120\kappa_2^{5/2}} + \frac{(i\lambda)^3}{6} \left(\xi_2 - \frac{3\xi_3}{2\kappa_2} \right) \right] + \dots \end{aligned} \quad (22)$$

Exponentiate the above equation, we have

$$\chi_M(\lambda; l) = \left(1 + \sum_{j=1}^{\infty} \frac{q_j(i\lambda)}{l^{j/2}} \right) e^{-\lambda^2/2} \quad (23)$$

where q_j is a polynomial of degree $3j$.

Finally, to obtain F_l in (13), we do the inverse Fourier transformation to get the probability density, and integrate it over x to get the probability distribution. Defining

$$\Phi(x) \equiv \int_{-\infty}^x \frac{dq}{\sqrt{2\pi}} e^{-\frac{1}{2}q^2} \quad (24)$$

to be the error function. We obtain:

$$F_l(x) = \Phi(x) + \sum_{j=1}^{\infty} \frac{q_j(-\partial_x)}{l^{j/2}} \Phi(x). \quad (25)$$

In general q_j is a complicated polynomial, which can be compute to all orders. Here we write explicitly the first few terms:

$$\begin{aligned} q_1 &= -\frac{\kappa_3(\partial_x)^3}{6\kappa_2^{3/2}} \\ q_2 &= \frac{\kappa_4(\partial_x)^4}{24\kappa_2^2} + \frac{\kappa_3^2(\partial_x)^6}{72\kappa_2^3} \\ q_3 &= -\frac{\kappa_3^3(\partial_x)^9}{1296\kappa_2^{9/2}} - \frac{\kappa_3\kappa_4(\partial_x)^7}{144\kappa_2^{7/2}} - \frac{\kappa_5(\partial_x)^5}{120\kappa_2^{5/2}} \\ &\quad - \frac{(\partial_x)^3}{6} \left(\xi_2 - \frac{3\xi_3}{2\kappa_2} \right) \end{aligned} \quad (26)$$

Comparing the above result with the usual Edgeworth series [20, 21], we find the first two terms are the same as those appearing in the Edgeworth expansion for l independent measures with cumulants κ_i , the correction from the boundary term χ_0 only effects the third and higher order terms.

It is important to note that the parameters κ_i, ξ_i are, in principle, measurable. For example, κ_2, ξ_2 can be obtained from the total noise in the measurement of l and $l+1$ spins as $\kappa_2 = \langle \Delta \mathcal{S}_{l+1}^2 \rangle - \langle \Delta \mathcal{S}_l^2 \rangle$ and $\xi_2 = (l+1)\langle \Delta \mathcal{S}_l^2 \rangle - l\langle \Delta \mathcal{S}_{l+1}^2 \rangle$, where $\Delta \mathcal{S}_l \equiv \mathcal{S}_l - \langle \mathcal{S}_l \rangle$.

Alternatively, by considering $\chi_0(\lambda)$ as a differential operator acting on the Fourier transform of χ_1 , and combining the Taylor series for $\chi_0(\lambda) = \sum_{k=0}^{\infty} \frac{f_k}{k!} \lambda^k$ with the Edgeworth series for χ_1^l , we may write explicitly

$$\tilde{F}_l = \text{Prob}\left(\frac{\mathcal{S}_l - l\kappa_1}{\sqrt{\kappa_2 l}} \leq x\right) = \sum_{L=0}^{\infty} \frac{1}{l^{L/2}} \sum_{m=0}^L \frac{i^m f_m \mathcal{G}_{L-m,m}}{\kappa_2^{m/2} m!} \quad (27)$$

where $\mathcal{G}_{k,m}(x)$ is given by $\mathcal{G}_{0,m} = (-\partial_x)^m \Phi(x)$:

$$\mathcal{G}_{k,m} = \sum_{\substack{\{p_1, \dots, p_k\} \in \mathbb{Z}_+^k \\ \sum p_i = k; \sum p_i = j}} \frac{(-\partial_x)^{k+m+2j} \Phi(x)}{p_1! \dots p_k!} \left(\frac{\kappa_3}{3!}\right)^{p_1} \dots \left(\frac{\kappa_{k+2}}{(k+2)!}\right)^{p_k}.$$

We can now compute F_l by using the expression (27), combined with:

$$F_l(x) = \text{Prob}\left(\frac{\mathcal{S}_l - l\mu(l)}{\sqrt{\text{var}(\mathcal{S}_l)/l}} \leq x\right) = \text{Prob}\left(\frac{\mathcal{S}_l - l\kappa_1}{\sqrt{\kappa_2 l}} \leq \frac{1}{\sqrt{1 + \frac{\xi_2}{l\kappa_2}}} x - \frac{\xi_1}{\sqrt{l\kappa_2}}\right) = \tilde{F}_l\left(\frac{1}{\sqrt{1 + \frac{\xi_2}{l\kappa_2}}} x - \frac{\xi_1}{\sqrt{l\kappa_2}}\right)$$

To illustrate these ideas, let us consider the following spin 1 MPS, given by the properly normalized matrices:

$$A^+ = \sqrt{\frac{1}{3}} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}; A^0 = \sqrt{\frac{1}{6}} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}; A^- = \sqrt{\frac{1}{3}} \begin{pmatrix} 0 & 0 \\ -1 & -1 \end{pmatrix}$$

Plugging these matrices in the definition (2) we find that:

$$E(\lambda) = \frac{1}{6} \begin{pmatrix} 2e^{i\lambda} + 1 & 2e^{i\lambda} - 1 & 2e^{i\lambda} - 1 & 2e^{i\lambda} + 1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 2e^{-i\lambda} + 1 & 2e^{-i\lambda} + 1 & 2e^{-i\lambda} + 1 & 2e^{-i\lambda} + 1 \end{pmatrix}$$

At $\lambda = 0$ we find that the largest eigenvalue is 1, and that it is separated by a gap from the next eigenvalue $1/3$.

In Fig 1. we compare the probability distribution for magnetization computed numerically from the ground state wave function, with the probability distribution obtained from our Edgeworth series (25). Here, the exact probability distribution $F_l(M)$ was found numerically by doing an inverse Fourier transformation of eq. (3). In the example depicted in Fig 1, for a block of 20 spins,

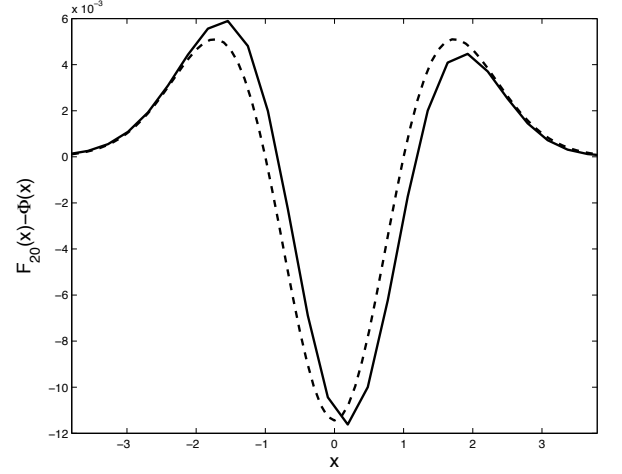


FIG. 1: Correction to the central limit distribution (i.e., $F_l(M) - \Phi(M)$). Solid line represent the exact result by calculating the probability distribution, dashed line shows the first order correction using Edgeworth series.

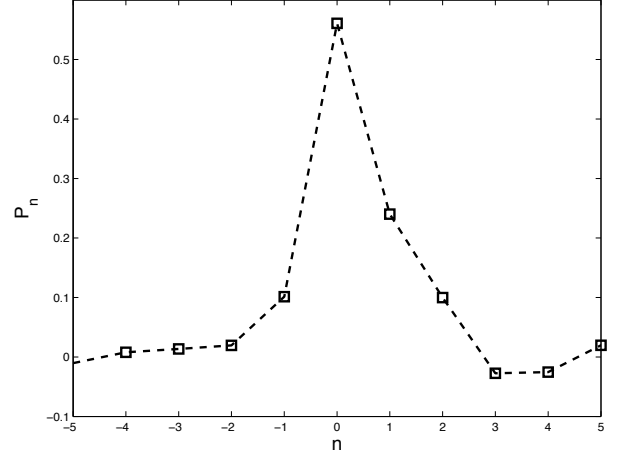


FIG. 2: First few Fourier components of χ_1 , showing small but finite negative pseudo-probabilities.

it is evident that the Edgeworth series works extremely well, capturing the essence of the correction already at first order. We also exhibit the pseudo-probabilities in Fig. 2, computed according to eq. (17).

Next, we consider an example where the full counting statistics is not described by a Gaussian of finite width, although the system is gapped. In this example, the variance *per site* actually vanishes as $1/l$. Consider the so called Affleck, Lieb, Kennedy and Tasaki (AKLT) state. The AKLT state [30] is a unique ground state of the AKLT Hamiltonian. It has a "string", instead of local, order parameter, and also fractionalized edge excitations. See [31, 32] for a more recent study. The AKLT Hamil-

tonian is,

$$\hat{H} = \sum_j \{ \mathbf{S}_j \mathbf{S}_{j+1} + \frac{1}{3} (\mathbf{S}_j + \mathbf{S}_{j+1})^2 \}.$$

The ground state has an MPS form, according to [33]

$$A^+ = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; A^0 = \sqrt{\frac{1}{3}} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; A^- = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$$

which gives:

$$E(\lambda) = \frac{1}{3} \begin{pmatrix} 1 & 0 & 0 & 2e^{i\lambda} \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 2e^{i\lambda} & 0 & 0 & 1 \end{pmatrix}.$$

Computing the eigenvalues of $E(\lambda)$, we see that they are $1, -\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}$, independent on λ . In the limit of $N, l \rightarrow \infty$, $e^S(\lambda, l, N) \rightarrow \frac{1+\cos\lambda}{2}$, we find that the counting statistics does not depend on l .

This result reflects the topological nature of the AKLT state, the total spin of the block depends only on the "edge modes" which are the only ones which are allowed to fluctuate.

In general, the absence of scaling of fluctuations, appears whenever we have a correspondence of the form

$$E(\lambda) = V(\lambda)E(0)V^{-1}(\lambda) \quad (28)$$

For some matrix V . In such a case, $\chi_1(\lambda) \equiv 1$, and the entire contribution comes from the edge $\chi(\lambda; l) = \chi_0(\lambda)$. In this case $\log \chi(\lambda)$ is clearly not extensive in the block size l .

To summarize, Matrix product states supply a very natural class of probability distribution which are not IID, but are still quite amenable to treatment and computation. In this paper we have studied the full counting statistics of spin in matrix product states. We explored the finite size correction to the Gaussian counting statistics expected on large scales. We showed how an Edgeworth type series may be used describe these asymptotic corrections and checked it numerically on an explicit example. Finally, we showed that in special cases, such as the AKLT model, the fluctuations in the system do not scale linearly with system size, and the Edgeworth description is not valid whenever it is based on variance and mean which were measured on any finite size block.

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